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Key indicators

Single-crystal X-ray study
 $T = 120\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.048
 wR factor = 0.119
Data-to-parameter ratio = 20.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

4-Iodotetrathiafulvalene–1,4-dinitrobenzene (1/1)

4-Iodotetrathiafulvalene and 1,4-dinitrobenzene form a 1:1
molecular complex, $\text{C}_6\text{H}_3\text{IS}_4 \cdot \text{C}_6\text{H}_4\text{N}_2\text{O}_4$. The structure
comprises mixed stacks of neutral molecules.

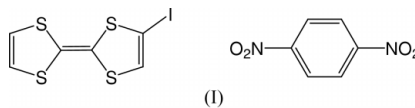
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Comment

The title complex, (I), was prepared in the course of our studies of charge-transfer (CT) systems involving halogenated derivatives of tetrathiafulvalene (TTF) (Batsanov *et al.*, 2001, and references therein). The structure contains mixed stacks (parallel to the b axis) of alternating molecules of the donor 4-iodotetrathiafulvalene (ITTF) and acceptor 1,4-dinitrobenzene (DNB), with an average interplanar separation of *ca* 3.5 Å (the molecules being not strictly parallel). The stacks are linked into 'double ribbons' by intermolecular (and inter-stack) contacts $\text{I} \cdots \text{O}_2^i$ [symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$] of 3.191 (4) Å, considerably shorter than the normal van der Waals contact distance of 3.61 Å (Rowland & Taylor, 1996) and probably corresponding to weak donor–acceptor interactions [see discussion and references in Batsanov *et al.* (2001)]. The $\text{C}2-\text{I} \cdots \text{O}2$ angle of 160.84 (15)° is consistent with this description.



The ITTF molecule shows essentially the same bond lengths as in the crystal structure of pure ITTF (Wang *et al.*, 1994), and widely different from those in $\text{ITTF}^{+\cdot}$ cation radicals (Batsanov *et al.*, 1997), indicating a virtual absence of intermolecular charge-transfer in (I) (Clemente & Marzotto, 1996). Likewise, bond distances in the DNB molecule coincide, within experimental error, with those in pure DNB (di Rienzo *et al.*, 1980; Tonogaki *et al.*, 1993).

The ITTF molecule in (I) adopts a slight boat conformation, folding along the $\text{S}1 \cdots \text{S}2$ and $\text{S}3 \cdots \text{S}4$ vectors by 4.39 (5) and 8.2 (1)°, respectively. The benzene ring of DNB is planar, and the nitro groups $\text{N}1/\text{O}1/\text{O}2$ and $\text{N}2/\text{O}3/\text{O}4$ are inclined to the ring plane by 7.4 (1) and 4.5 (2)°, respectively.

Experimental

ITTF (8.7 mg, 0.0263 mmol) was added to DNB (4.5 mg, 0.0268 mmol) dissolved in hot chloroform (1.2 ml) and stirred until fully dissolved. The solution was left at room temperature for several days, allowing very slow evaporation of the solvent. Green X-ray quality crystals of (I) formed. Elemental analysis confirmed the 1:1 composition. Found: C 29.21, H 1.52, N 5.85%; calculated for $\text{C}_{12}\text{H}_7\text{IN}_2\text{O}_4\text{S}_4$: C 28.92, H 1.42, N 5.62%.

Crystal data

$C_6H_3IS_4 \cdot C_6H_4N_2O_4$
 $M_r = 498.34$
 Monoclinic, $P2_1/c$
 $a = 18.926$ (4) Å
 $b = 7.096$ (1) Å
 $c = 12.450$ (3) Å
 $\beta = 105.93$ (2)°
 $V = 1607.8$ (6) Å³
 $Z = 4$

$D_x = 2.059$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 763 reflections
 $\theta = 11.9$ – 23.4 °
 $\mu = 2.53$ mm⁻¹
 $T = 120$ (2) K
 Plate, dark green
 $0.34 \times 0.18 \times 0.01$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
 ω scans
 Absorption correction: by integration (*XPREP* in *SHELXTL*; Bruker, 1998)
 $T_{\min} = 0.558$, $T_{\max} = 0.974$
 12107 measured reflections

4254 independent reflections
 2903 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$
 $\theta_{\text{max}} = 29.2$ °
 $h = -17 \rightarrow 25$
 $k = -9 \rightarrow 9$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.119$
 $S = 1.02$
 4254 reflections
 208 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0635P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.61$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.96$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

I—C2	2.085 (5)	O1—N1	1.221 (6)
S1—C2	1.743 (5)	O2—N1	1.227 (6)
S1—C1	1.765 (5)	O3—N2	1.229 (6)
S2—C3	1.736 (5)	O4—N2	1.219 (6)
S2—C1	1.763 (5)	N1—C11	1.469 (7)
S3—C5	1.736 (6)	N2—C14	1.481 (7)
S3—C4	1.755 (5)	C11—C16	1.393 (7)
S4—C6	1.746 (6)	C11—C12	1.394 (7)
S4—C4	1.759 (5)	C12—C13	1.379 (8)
C1—C4	1.357 (7)	C13—C14	1.368 (8)
C2—C3	1.348 (7)	C14—C15	1.406 (7)
C5—C6	1.338 (9)	C15—C16	1.374 (7)
C2—S1—C1	94.3 (2)	O1—N1—O2	124.3 (5)
C3—S2—C1	95.3 (3)	O1—N1—C11	118.8 (5)
C5—S3—C4	94.7 (3)	O2—N1—C11	117.0 (4)
C6—S4—C4	94.4 (3)	O4—N2—O3	125.4 (5)
C4—C1—S2	120.9 (4)	O4—N2—C14	117.6 (5)
C4—C1—S1	124.4 (4)	O3—N2—C14	117.0 (5)
S2—C1—S1	114.7 (3)	C16—C11—C12	122.7 (5)
C3—C2—S1	118.6 (4)	C16—C11—N1	118.6 (5)
C3—C2—I	122.8 (4)	C12—C11—N1	118.6 (4)
S1—C2—I	118.6 (3)	C13—C12—C11	117.9 (5)
C2—C3—S2	117.0 (4)	C14—C13—C12	119.8 (5)
C1—C4—S3	124.2 (4)	C13—C14—C15	122.4 (5)
C1—C4—S4	120.9 (4)	C13—C14—N2	119.3 (5)
S3—C4—S4	114.9 (3)	C15—C14—N2	118.3 (5)
C6—C5—S3	117.9 (5)	C16—C15—C14	118.4 (5)
C5—C6—S4	117.7 (5)	C15—C16—C11	118.7 (5)

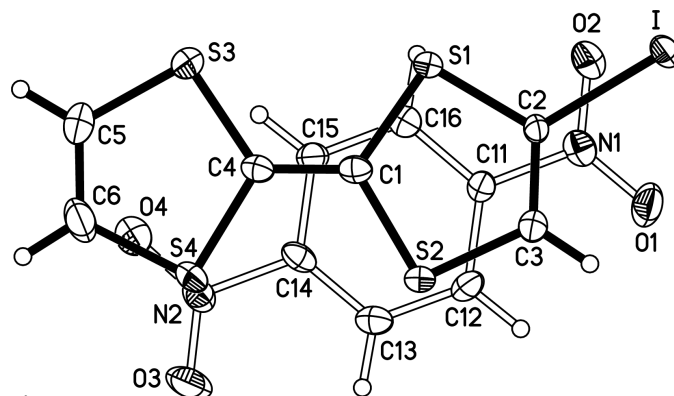


Figure 1

The 4-iodotetrathiafulvalene and 1,4-dinitrobenzene molecules in (I). Atomic displacement ellipsoids are shown at the 50% probability level.

All H atoms were located in a difference Fourier synthesis, but were then treated as riding in idealized positions ($C-H = 0.95$ Å). The largest peak and deepest hole were located 0.91 and 0.84 Å, respectively, from the I atom.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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